Qualitative Tier 2 Assessment

Alkanes, C11-15-iso-

In accordance with the Chemical Risk Assessment Framework (CRAF), chemicals assigned a Tier 2 designation require a hazard assessment and qualitative assessment of risk.

Consistent with National Industrial Chemicals Notification and Assessment Scheme (NICNAS), the human health hazards for each chemical are characterised by analysing the toxicokinetics (the absorption, distribution, metabolism and excretion of the chemical in humans or laboratory animals), acute toxicity, irritation and corrosivity, repeat dose toxicity, genotoxicity, carcinogenicity, reproductive toxicity, and other health effects. The environmental hazards for each chemical are characterized by analysing the environmental fate properties (such as mobility, persistence, bioavailability and bioaccumulation), acute toxicity and chronic toxicity. In support of the hazard assessment, a risk assessment dossier is prepared for each of the chemicals included in the assessment.

The qualitative assessment of risk evaluates exposure to the vendor chemical that may occur during activities that do not intentionally result in a release to the environment, but where a potential release may occur. For this evaluation, these potential releases primarily are focused on the vendor chemical transported to the well pad site or water management facility (WMF), chemicals utilised in drilling fluid systems that may impact groundwater, residual chemicals that may be present in hydraulic flowback and workover fluids and chemicals and chemicals and residues of chemicals that may be present in water undergoing treatment or beneficially re-used.

Potentially complete exposure pathways (in that a source, a migration pathway, a mechanism for exposure, and a potential receptor are present) are assessed herein to determine the potential for risk (an incomplete pathway precludes an exposure occurring and an associated potential risk). In this context, site setting and management protocols associated with the action are evaluated. Key controls limiting the potential for exposure include:

- Engineering controls (including fencing and secondary containment);
- Storage (drums, totes and storage tanks) constructed in accordance with Australian standards and managed and monitored in accordance with regulatory requirements;
- Maintenance of access control restrictions during site activities that will preclude access by the public, livestock and large native fauna; and,
- Australia SafeWork Place and Santos Occupational Safety Guidance used to minimise human health exposure.

As a result, the assessment for this Tier 2 chemical includes the following components: completing the screening; developing a risk assessment dossier and Predicted No Effect Concentrations (PNECs) for water and soil; and, providing a qualitative discussion of risk. Each of these components is detailed within this memorandum.

Background

Alkanes, C11-C15-iso is a chemical in a workover product used in hydraulic fracturing activities. The workover process is designed to remove any solids from the well and facilitate placement of the pump. As part of this process, fluids and some coal fines are removed from the well and transported to produced water ponds for management within produced water stream. Once the well has been placed and commissioned, flowback and produced water is discharged into the water gathering pipelines and conveyed to the water ponds/water treatment facilities for treatment and beneficial use (such as dust suppression, construction, operational use and stock water for cattle).

The purpose and maximum quantity for this chemical is summarised in **Table 1**.

Table 1 Initial and Underbalance Workover Fluid Chemicals

Chemical Name	CAS No.	Use	Quantity[1]
Alkanes, C11-15-iso-	90622-58-5	Activators, Emulsifiers and Neutralisers	NA

[1] Volume Percent in Treatment (%)
CAS No = Chemical Abstracts Service Number
NA = quantity used varies

No data on alkanes, C11-15-iso- were located. Data for this dossier has been read-across from similar hydrocarbon substances and from the C9-C14 aliphatic (≤2% aromatics) hydrocarbons solvents category used for the European Union Registration, Evaluation, Authorisation and Restriction of Chemicals (EU REACH). The assessment of toxicity of this chemical was used to evaluate human health exposure scenarios and is presented in **Attachment 1**. There are no carcinogenicity studies on C9-C14 aliphatic (≤2% aromatics) and, as a result, only a non-carcinogenic oral reference dose (RfD) was calculated. A detailed discussion of the derivation of the oral RfD and drinking water guideline values is presented in **Attachment 1**. **Table 2** provides a summary of the derivation.

Table 2 Oral Reference Doses and Derived Drinking Water Guidelines

Constituent (CAS No.)	Study	Critical Effect/ Target Organ(s)	NOAEL (mg/kg-day)	Uncertainty Factors	Oral Reference Dose (mg/kg-day)	Drinking Water Guideline (mg/L)
Alkanes, C11-15-iso- (90622-58-5)	Reproductive/ Developmental Study	None	1000	300	3.33	12

Refer to **Attachment 1** for information on the key studies selected for oral reference dose and drinking water level development.
CAS = Chemical Abstracts Service
mg/kg-day = milligram per kilogram-day
mg/L = milligram per litre
NOAEL = No observed adverse effect level

For ecological receptors, the assessment utilises the information presented in the dossiers on the relative toxicity of the aquatic and terrestrial flora and fauna to the chemical. This assessment focuses on the aquatic invertebrate and fish species within the surface water resources and the soil flora and fauna associated with releases to the soil.

The determination of toxicological reference values (TRVs) was conducted according to the PNEC guidance in the *Environmental Risk Assessment Guidance Manual for Industrial Chemicals* prepared by the Australian Environmental Agency (AEA, 2009). PNECs for freshwater and sediment were developed to assess aquatic receptors, and PNECs for soil were developed for terrestrial receptors.

Table 3 present the chemical, the endpoint, no observable effects concentration (NOEC) (milligrams per litre [mg/L]), assessment factor, and the aquatic PNEC (mg/L). PNECs for sediment and soil are detailed in **Tables 4** and **5,** respectively. Refer to **Attachment 1** for the development of PNECs, or the rational for PNECs that do not have a calculated PNEC.

Table 3 PNECs Water – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/L)	Assessment Factor	$PNEC_{water}$ (mg/L)
Alkanes, C11-15-iso- (90622-58-5)	-	-	-	0.001[a]

[a] PNEC estimated using the quantitative structure activity relationship (QSAR) model PETRORISK v7.04.
EC_{50} = effects concentration – 50%
mg/L = milligram per litre
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 4 PNECs Sediment – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg wet wt)	Assessment Factor	$PNEC_{sed}$ (mg/kg wet wt)
Alkanes, C11-15-iso- (90622-58-5)	[a]	-	-	260

[a] PNEC estimated using the quantitative structure activity relationship (QSAR) model PETRORISK v7.04
EC_{50} = effects concentration – 50%
mg/kg wet wt = milligram per kilogram wet weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 5 PNECs Soil – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg dry wt)	Assessment Factor	$PNEC_{soil}$ (mg/kg dry wt)
Alkanes, C11-15-iso- (90622-58-5)	[a]	-	-	100

[a] PNEC estimated using the quantitative structure activity relationship (QSAR) model PETRORISK v7.04
EC_{50} = effects concentration – 50%
mg/kg dry wt = milligram per kilogram dry weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

A detailed assessment of the risks posed by this Tier 2 chemical is provided in the following sections.

General Overview

The C11-C15 iso alkanes are comprised of complex aliphatic hydrocarbon solvents that contain >98% aliphatic constituents with carbon numbers in the range of C11-C15 and less than 2% aromatic constituents. The chemical constituents in this complex Unknown or Variable Composition, Complex Reaction Products and Biological Materials (UVCB) substance may include straight chain (n-), branched (iso-) and cyclic aliphatic hydrocarbons but have less than 2% aromatic hydrocarbons. The molecular structure of alkanes, C11-15-iso is presented in **Figure 1**.

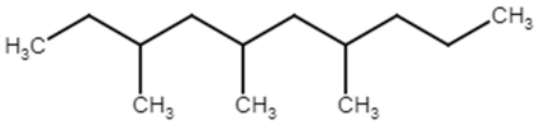

Figure 1 Molecular Structure of Alkanes, C11-15-iso[1]

Aliphatic hydrocarbons composed of branched (isoalkanes) and cyclic aliphatic hydrocarbons in the C10 to C16 range have reported to be readily biodegradable to not inherently biodegradable. The alkanes, C11-15-iso- are expected to highly absorb to sediment and soil. Alkanes, C11-15- iso- is expected to have constituents with the potential to bioaccumulate.

The Persistent, Bioaccumulative and Toxic (PBT) assessment for alkanes, C11-15-iso is included in the dossier provided in **Attachment 1**. Based on physico-chemical properties and screening data detailed below, the overall conclusion was that alkanes, C11-15-iso is not a PBT substance.

[1] Source https://chem.nlm.nih.gov/chemidplus/rn/90622-58-5

Human Health Hazards

The acute toxicity of C9-C14 aliphatic hydrocarbons (≤2% aromatics), which includes the alkanes, C11-15-iso-, is low by the oral, dermal and inhalation route. It is, however, an aspiration hazard. C9-C14 aliphatic hydrocarbons (≤2% aromatics) are not skin or eye irritants or a dermal sensitiser.

Repeated inhalation exposure of rats to a C9-C14 aliphatic, ≤2% aromatic hydrocarbon fluid showed no target organ effects; oral exposures to very high doses of these hydrocarbons showed irritation to the gastrointestinal tract and effects in the liver that likely represent an adaptive response to the metabolism of the hydrocarbons and not a toxic response. C9-C14 aliphatic hydrocarbons (≤2% aromatics) are not genotoxic; nor do they exhibit any evidence of reproductive or developmental toxicity in rats.

A reproductive/developmental toxicity study was conducted on a C9-C14 aliphatic (<2% aromatic) hydrocarbon fluid in rats. There were no adverse effects at 1,000 milligrams per kilogram-day (mg/kg-day), the highest dose tested. The no observed adverse effect level (NOAEL) of 1,000 mg/kg-day was used to derive the oral RfD and the drinking water guideline value (12 milligrams per litre [mg/L]) (see **Table 2**). Description of the oral RFD and calculation of the drinking water guideline value is included in the dossier provided in **Attachment 1**.

The lifecycle of chemicals, including alkanes, C11-15-iso, used during the hydraulic fracturing of wells includes the following general categories: transportation of chemicals; hydraulic fracturing activities; and, treatment, recycling, disposal and beneficial reuse. Without management controls in place, there is the potential for human receptors to be exposed to alkanes, C11-15-iso in hydraulic fracturing workover chemicals during stimulation and completion operations and management of flowback and work-over fluids and during beneficial re-use. Based on an assessment of land use and an understanding of the project description provided in the Environmental Impact Statement (EIS) (URS, 2014) and the CRAF developed for the GFD Project Area, potential human receptors include:

1. Workers at the well lease involved with: blending, injection and recovery of hydraulic fracturing and work-over fluids; recycling, reuse or disposal of recovered fluids including beneficial reuse activities such as land applications of drilling materials and dust suppression; and, mitigating releases from the well lease to an adjacent water body.
2. Agricultural workers/residents at irrigation areas.

In terms of risks associated with transport of chemicals and wastes, this risk is considered to be managed to a level as low as reasonably practicable. This is because the potential for a release is controlled through implementation of traffic management principles including use of designated trucking routes, vehicle signage, vehicle management systems (to manage speed and driving behaviour/habits) and, in the unlikely event of a vehicular accident, implementation of incident and spill response procedures. Given the highly regulated nature of transportation of chemicals (at both a Commonwealth and State level), transport-related scenarios are not evaluated further in this assessment. However, the outcome of the assessment should be used to inform emergency response actions.

Unlike drilling there are no large volumes of premixed stimulation fluid systems stored on-site. The primary fluid stored on-site is water, and chemicals are blended into the fluid stream as it is used. Exposure of workers to stimulation fluid chemicals is possible via inadvertent spills and leaks, during the recycling and beneficial reuse of recovered materials (e.g., drilling fluids and cuttings), and during application of the recovered material to land. However, chemical exposures to workers are

controlled through engineering, management controls and personal protective equipment, which are focused on elimination and mitigation of the potential for dermal contact and incidental ingestion. In addition, Australia SafeWork Place and Santos Occupational Safety Guidance are used to minimise human health exposure. As a result, petroleum workers, are also excluded from assessment. No potentially complete exposure pathways were identified.

In the unlikely event of a release to ground at the well lease, the potential for exposures (other than workers) is limited. The well pad sites are fenced and access is controlled, which limits access to the public. If stimulation fluid chemicals are spilled to ground, then investigation, remediation and rehabilitation activities would be implemented to address soil impacts.

On-lease storage may utilise tanks, pits or turkey nests and there is the possibility that a containment failure could result in the release of the materials to the well lease and the surrounding environment. Releases on the well pad would be of limited volumes and, as such, these products would not be anticipated to migrate a significant distance off lease to the surrounding environment, including proximal water bodies. Releases from the gathering pipeline would be of higher potential volumes but the flow back or workover fluid concentrations from an individual well would be diluted with other waters from other wells also flowing in this gathering network.

Exposure of potential receptors (other than workers) is also possible to residual chemicals in areas adjacent to a well lease that have been used for the application of materials for beneficial reuse. The primary land use within the development area is agricultural (grazing on improved or unimproved pastures), and it is sparsely populated. There may be potential for human receptors such as residents and agricultural workers to be exposed to residual chemicals in ponded irrigation water or irrigated soil via direct contact (ingestion and dermal) and inhalation pathways. Relative potential exposure to agricultural workers/residents is considered low due to the remote location of the well leases and the sparse population. In addition, activities are undertaken in operational and controlled areas of the well lease.

However, Environmental Authority (EA) or Beneficial Use Approval conditions regulate project reuse. A plan for the beneficial reuse of materials has been developed by a Suitably Qualified Person (SQP) in accordance with the EA conditions which require materials of a certain quality and controls the maximum volumes that can be applied to land. In addition, the application techniques and location of application are controlled with specific monitoring required. Irrigation areas are designed to manage the risk of pooling and run-off with a general deficit irrigation strategy employed; and, are fitted with monitoring bores to manage the risk of vertical and horizontal migration. Additional details regarding mitigation and management controls are discussed in the CRAF.

As a result, potential exposures during stimulation and workover activities is considered low due to the employment of mechanical equipment/processes, engineering controls (including secondary containment) and other mitigation and management strategies. Similarly, there is a low potential for human receptors exposed to residual chemicals in areas adjacent to a well lease that have been used for the application of materials for beneficial reuse and to surface water bodies that may receive runoff from beneficial reuse applications. Finally, the probability of any surface related discharge infiltrating subsurface soils and migrating to groundwater is very low.

Environmental Hazards

Based on an evaluation of aquatic toxicity tests in similar hydrocarbons, alkanes, C11-15-iso- has a low acute toxicity concern to aquatic life. Acute toxicity towards aquatic invertebrates and algae is of the same order of magnitude. However, fish were more sensitive in chronic toxicity testing (ECHA).

Alkanes, C11-15-iso is not expected to be readily biodegradable and contains constituents that have the potential to bioaccumulate.

PNECs for alkanes, C11-15-iso are provided in **Tables 3 – 5**. As noted in the tables, there are no toxicity data for sediment-dwelling organisms or soil organisms. Therefore, PNECs for sediment and soil were calculated using the quantitative structure activity relationship (QSAR) model PETRORISK v7.04. The QSAR model was also used to calculate a PNEC for water. PNEC calculations and assumptions are included in the dossier provided in **Attachment 1**.

During the hydraulic fracturing process, there is the potential for environmental receptors to be exposed to workover fluid chemicals such as alkanes, C11-15-iso. Pipelines (where treated water is conveyed) can transect sensitive ecological areas (including Matters of National Environmental Significance [MNES]). There is the concern of wildlife (terrestrial and aquatic receptors) and livestock in the vicinity of the well leases to have adverse effects from potential exposures. Potential environmental receptors include:

1. Wildlife and livestock accessing the well lease and areas adjacent to a well lease, including surface water features that have received runoff from an accidental release during hydraulic fracturing activities or loss of containment.
2. Wildlife and livestock accessing areas of the well lease where materials have been applied as well as accessing stored materials in pits and turkey nests.
3. Aquatic flora and fauna within a proximal surface water body that has received runoff from an accidental release during hydraulic fracturing activities or loss of containment, or from beneficial use applications.
4. Wildlife including livestock that have access to the water supply from a bore hydraulically downgradient of the well lease.

The potential for exposure of sensitive receptors (including [MNES) is considered low. The hydraulic fracturing activities occur over a short duration and are conducted in controlled/operational areas within a perimeter fence. Further, the activity level, noise, etc. will be a disincentive for wildlife and livestock to access the lease through gaps in the fencing or unsecured gates.

Based on the engineering and management controls described in the previous section (Human Health Hazards), there is a low potential for ecological receptors exposed to surface water bodies that may receive runoff from an accidental release. There is also concern that recovered material applied to the land surface could migrate to groundwater or surface water, and therefore result in adverse effects to the environment (e.g., uptake by aquatic receptors). Due to EA conditions regulating land application techniques, the remote nature of the well leases, vertical separation of groundwater and distances to watercourses, the ephemeral nature of the watercourses and the physical and chemical properties of the residual chemicals post treatment or beneficial reuse, these potential exposures are also low.

References

Australian Environmental Agency (AEA). (2009). Environmental Risk Assessment Guidance Manual for Industrial Chemicals, Commonwealth of Australia.

ECHA. ECHA REACH database: http://echa.europa.eu/information-on-chemicals/registered-substances

URS. (2014). Santos GLNG Project: Gas Field Development Project Environmental Impact Statement. Available online at: http://www.santosglng.com/environment-and-water/gas-field-development-project-eis.aspx

Attachment 1 Risk Assessment Dossier

ALKANES, C11-15-ISO-

This dossier on alkanes, C11-15-iso- presents the most critical studies pertinent to the risk assessment of alkanes, C11-15-iso- in its use in coal seam gas extraction activities. It does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained primarily from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Alkanes, C11-15-iso- was not identified in chemical databases used by NICNAS as an indicator that the chemical is of concern and is not a PBT substance. Alkanes, C11-15-iso- was assessed as a tier 2 chemical for chronic toxicity. Therefore, alkanes, C11-15-iso- is classified overall as a **tier 2** chemical and requires a hazard assessment and qualitative assessment of risk.

1 BACKGROUND

The C11-C15-iso- alkanes are comprised of complex aliphatic hydrocarbon solvents that contain >98% aliphatic constituents with carbon numbers in the range of C11-C15 and less than 2% aromatic constituents. The chemical constituents in this complex UVCB substance may include straight chain (n-), branched (iso-) and cyclic aliphatic hydrocarbons but have less than 2% aromatic hydrocarbons.

Aliphatic hydrocarbons composed of branched (isoalkanes) and cyclic aliphatic hydrocarbons in the C10 to C16 range have reported to be readily biodegradable to not inherently biodegradable. Members of this group are insoluble and are expected to highly adsorb to sediment and soil. Based on similar substance, C11-C15-iso- alkanes are not expected to bioaccumulate and have a low acute toxicity concern to aquatic life.

The acute toxicity of similar substance C9-C14 aliphatic hydrocarbons (≤2% aromatics), which includes the alkanes, C11-15-iso-, is low by the oral, dermal and inhalation route. It is, however, an aspiration hazard. C9-C14 aliphatic hydrocarbons (≤2% aromatics) are not skin or eye irritants or a dermal sensitiser. Repeated inhalation exposure of rats to a C9-C14 aliphatic, ≤2% aromatic hydrocarbon fluid showed no target organ effects; oral exposures to very high doses of these hydrocarbons showed irritation to the gastrointestinal tract and effects in the liver that likely represent an adaptive response to the metabolism of the hydrocarbons and not a toxic response. C9-C14 aliphatic hydrocarbons (≤2% aromatics) are not genotoxic; nor do they exhibit any evidence of reproductive or developmental toxicity in rats.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Alkanes, C11-15-iso-
CAS RN: 90622-58-5
Molecular formula: Not available (UVCB substance)
Molecular weight: Not available (UVCB substance)
Synonyms: Alkanes, C11-15-iso-; C11-15 isoalkanes

3 PHYSICO-CHEMICAL PROPERTIES

Physical and chemical properties were not available for the UVCB hydrocarbon. As a result, information was obtained from a read-across substance (alkanes, C12-14-iso-). Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Alkanes, C12-14-iso- (CAS No. 68551-19-9)

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Colourless liquid with a faint odour	2	ECHA
Melting point	-114°C @ 101.3 kPa (pour point)	2	ECHA
Boiling point	189 to 206°C @ 101.3 kPa	2	ECHA
Density	760 kg/m^3 @ 15°C	2	ECHA
Vapour pressure	40 Pa @ 20°C	2	ECHA
Partition coefficient (log K_{ow})	5.94 to 7.14 (pH and temperature not calculated)	-	ECHA
Water solubility	0.00001 to 0.00015 g/L	-	ECHA
Viscosity	1.77 mm^2/s @ 20°C	2	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No other specific environmental regulatory controls or concerns were identified within Australia and internationally for alkanes, C11-15-iso-.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Aliphatic hydrocarbons composed of branched (isoalkanes) and cyclic aliphatic hydrocarbons in the C10 to C16 range have reported to be readily biodegradable to not inherently biodegradable. The alkanes, C11-15-iso- are insoluble and are expected to highly adsorb to sediment and soil. They are not expected to bioaccumulate.

B. Partitioning

Based on Henry's Law Constant values > 4.76 x 10^4 Pa-m^3/mol @25 °C, members of this group have the potential to volatilize from water or moist soil surfaces. These chemicals are unlikely to degrade by hydrolysis as they lack a functional group that is hydrolytically reactive. However, in the air, category members have the potential to rapidly degrade through indirect photolytic processes (OECD, 2012).

C. Biodegradation

In an OECD 301F test, hydrocarbons, C10-C13, isoalkanes, cyclics (<2% aromatics) degraded 89.8% after 28 days, indicating ready biodegradation (ECHA) [Kl. score = 2].

In an OECD 301F test, hydrocarbons C12-16, isoalkanes, cyclics (<2% aromatics) degraded 22% after 28 days and 50% after 70 days, indicating inherent biodegradation (ECHA) [Kl. score 2].

In a USEPA OTS 796.3100 aerobic aquatic biodegradation test, hydrocarbons, C13-C15, isoalkanes, cyclics (<2% aromatics) degraded 16.95% after 24 days and 20.62% after 31 days, indicating that it is not inherently but ultimately biodegradable (ECHA) [Kl. score = 2].

In a USEPA OTS 796.3100 aerobic aquatic biodegradation test, hydrocarbons, C12-C13, isoalkanes, cyclics (<2% aromatics) degraded 12.69% after 24 days and 13.69% after 31 days, indicating that it is not inherently but ultimately biodegradable (ECHA) [Kl. score = 2].

Overall, alkanes, C11-15-iso- are expected to ultimately biodegrade in the environment. If a chemical is found to be inherently or readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

D. Environmental Distribution

Alkanes, C11-15-iso- is a UVCB substance. The standard tests to determine the K_{oc} are for single substances and not for UVCB substances. Therefore, a K_{oc} value for C11-15-iso- was not determined.

The calculated K_{oc} values for linear aliphatic hydrocarbons dodecane and tetradecane are 110,000 and 759,000 L/kg, respectively, using SPARC v4.2 program in the CONCAWE Library of PETRORISK (ECHA). This modelled range of K_{oc} values are consistent with those presented in the review of C10 – C12 aliphatics by TPHCWG (1997). These values, along with the low solubility of substances in this group, suggest that alkanes, C11-15-iso- will highly adsorb to sediment and soil.

E. Bioaccumulation

Alkanes, C11-15-iso- is a UVCB substance. The calculated BCF values for linear aliphatic compounds undecane (C11), dodecane (C12), and tetradecane (C14) are 337.8, 790.9, and 962.9 L/kg, respectively, using the BCFWIN V2.16 model within EPISuite 3.12. The predicted BCFs for hydrocarbons are considered to be generally overly conservative because biotransformation is not quantitatively taken into account. For these linear aliphatic hydrocarbons, based on BCFs for indicator compounds - the values indicate that they are not expected to bioaccumulate.

6 HUMAN HEALTH HAZARD ASSESSMENT

A. Summary

The acute toxicity of C9-C14 aliphatic hydrocarbons (≤2% aromatics), which includes the alkanes, C11-15-iso-, is low by the oral, dermal and inhalation route. It is, however, an aspiration hazard. C9-C14 aliphatic hydrocarbons (≤2% aromatics) are not skin or eye irritants or a dermal sensitiser. Repeated inhalation exposure of rats to a C9-C14 aliphatic, ≤2% aromatic hydrocarbon fluid showed no target organ effects; oral exposures to very high doses of these hydrocarbons showed irritation to the gastrointestinal tract and effects in the liver that likely represent an adaptive response to the metabolism of the hydrocarbons and not a toxic response. C9-C14 aliphatic hydrocarbons (≤2% aromatics) are not genotoxic; nor do they exhibit and evidence of reproductive or developmental toxicity in rats.

B. Acute Toxicity

The oral LD_{50} in rats for C9-C14 aliphatic, ≤2% aromatic hydrocarbon fluids is >5,000 mg/kg (ECHA) [Kl. score = 2].

The 4-hour inhalation LC_{50} in rats for C9-C14 aliphatic, ≤2% aromatic hydrocarbon fluids is > 4,951 mg/m^3 [ECHA) [Kl. scores =1 and 2].

The dermal LD_{50} in rats for C9-C14 aliphatic, ≤2% aromatic hydrocarbon fluids is >5,000 mg/kg (ECHA) [Kl. score = 2].

C. Irritation

The C9-C14 aliphatic, ≤2% aromatic hydrocarbon fluids are neither skin nor eye irritants (ECHA) [Kl. scores = 1 and 2].

D. Sensitisation

C9-C14 aliphatic, <2% aromatic hydrocarbon fluids were not skin sensitisers when tested in guinea pig maximisation tests (ECHA) [Kl. score = 2].

A C9-C14 aliphatic, <2% aromatic hydrocarbon fluid showed no indication of skin sensitisation in a human repeated insult patch test (ECHA).

E. Repeated Dose Toxicity

Oral

Male and female rats were dosed by oral gavage with 0, 500, 2,500 or 5,000 mg/kg with a C9- C14 aliphatic (<2% aromatic) hydrocarbon fluid 7 days/week for 13 weeks. Additional groups of animals were dosed with 0 or 5,000 mg/kg for 13 weeks, followed by a 4-week recovery period. There were dose-related changes in the hematology and serum chemistry parameters which were consistent with changes seen in the liver. Hepatocellular hypertrophy (liver cell enlargement) were seen in both males and females in all dose groups and were reversible. The liver effects were not considered to be an indication of toxicity but an adaptive response due to the metabolism of the hydrocarbons. There were also mucosal thickening and other signs of irritation to the stomach and anus, which appeared to be the direct result of high-dose intubation of a locally irritating material. All treatment-related effects were reversible within the 4-week recovery period. The NOAEL for systemic effects in this study is considered to be 5,000 mg/kg-day (ECHA) [Kl. score = 1].

Hydrocarbons C11-C14, n-alkanes, isoalkanes, cyclics (<2% aromatics) (CAS RN 64742-47-8). Tested in a 90 day repeated oral toxicity test (OECD TG 408) in Sprague Dawley rats. The study design included a 28 day recovery period for rats exposed to the highest dose (1000 mg/kg/day). The NOAEL was 1000 mg/kg/day (OECD 2012) [Kl Score = 2].

Hydrocarbons C10-C12 isoalkanes (<2% aromatics) (CAS RN 64742-47-8). Tested in a 90 day repeated oral toxicity test (OECD TG 408) in Sprague-Dawley rats. The study design included a 28 day recovery period for rats exposed to the highest dose (1000 mg/kg/day). The NOAEL was 1000 mg/kg/day (OECD 2012) [Kl Score = 2].

Inhalation

Male and female rats were exposed by inhalation to 0, 2,600, 5,200, or 10,400 mg/m^3 of a C9-C14 aliphatic (<2% aromatic) hydrocarbon fluid, 6 hours/day, 5 days/week for 13 weeks. There were no mortality or effects in either the hematology or the serum chemistry parameters. The male rats at all dose levels had increased liver and kidney weights; male heart weights were also increased at 10,400 mg/m^3 and kidney weights were increased in the 10,400 mg/m^3 group. Kidney effects indicative of alpha-2u-globulin nephropathy were observed at all dose levels. There were no other effects that were considered to be treatment-related. The alpha-2u-nephropathy in the male rats are not considered to be relevant to humans; for the organ weight changes other than the male kidneys, there were no corresponding histopathologic changes. The NOAEL for this study is 10,400 mg/m^3, the highest exposure concentration tested (ECHA) [Kl. score = 1].

Dermal

No studies are available.

F. Genotoxicity

In Vitro Studies

The key *in vitro* genotoxicity studies on C9-C14 aliphatic hydrocarbons (≤2% aromatics) are presented in Table 3.

Table 3 In vitro Genotoxicity Studies on C9-C14 Aliphatic Hydrocarbons (≤2% Aromatics)

Test System	Results*		Klimisch Score	Reference
	-S9	+S9		
Bacterial reverse mutation (*S. typhimurium* and *E. coli* strains)	-	-	1	ECHA
Mammalian cell gene mutation (Chinese hamster V 79 cells)	-	-	2	ECHA
Chromosomal aberration (human lymphocytes)	-	-	1	ECHA

*+, positive; -, negative

In Vivo Studies

In two separate studies involving two different C9-C14 aliphatic (<2% aromatic) hydrocarbon fluids, male and female CD-1 mice were given a single oral gavage dose at concentrations of 0, 1,250, 2,500, or 5,000 mg/kg. The frequency of micronucleated polychromatic erythrocytes was not significantly increased in the treated mice compared to that in the controls (ECHA) [Kl. Score = 1].

In two separate dominant lethal studies involving two different C9-C14 aliphatic (<2% aromatic) hydrocarbon fluids, male rats were exposed 6 hours/day for 5 consecutive days to exposure concentrations of 0, 300, or 900 ppm. There was no evidence of a mutagenic response in the treated rats (ECHA) [Kl. score = 2].

G. Carcinogenicity

No carcinogenicity studies are available on the C9-C14 aliphatic (<2% aromatic) hydrocarbon fluids.

H. Reproductive Toxicity

A C9-C14 aliphatic (<2% aromatic) hydrocarbon fluid was tested in a combined repeated dose toxicity study with a reproductive/developmental toxicity screening test (OECD 422). Male and female SD rats were given oral gavage doses of 0, 25, 150, or 1,000 mg/kg-day. There was no indication of reproductive toxicity at any dose level. The NOAEL for reproductive toxicity is 1,000 mg/kg-day, the highest dose tested (ECHA) [Kl. score = 1].

A C9-C14 aliphatic, <2% aromatic hydrocarbon fluid was tested in a reproductive/developmental toxicity screening test (OECD 421). Male and female SD rats were given oral gavage doses of 0, 100, 300, or 1,000 mg/kg-day. There was no indication of reproductive toxicity or any effects on the endocrine system at any dose level. The NOAEL for reproductive toxicity is 1,000 mg/kg-day, the highest dose tested (ECHA) [Kl. score = 1].

I. Developmental Toxicity

A C9-C14 aliphatic (<2% aromatic) hydrocarbon fluid was tested in a rat pre-natal developmental toxicity study. Pregnant female rats were exposed by inhalation to 0, 300 or 900 ppm for 6

hours/day during gestation days 6 to 15. There was no evidence of maternal or developmental toxicity at either exposure level. The NOAEL for this study is 900 ppm (ECHA) [Kl. score = 1].

Another C9-C14 aliphatic, <2% aromatic hydrocarbon fluid was tested in a rat pre-natal developmental toxicity study. Pregnant female rats were exposed by inhalation to 0, 300 or 900 ppm for 6 hours/day during gestation days 6 to 15. There was no evidence of maternal or developmental toxicity at either exposure level. The NOAEL for this study is 900 ppm (ECHA) [Kl. score = 1].

J. Derivation of Toxicological Reference and Drinking Water Guidance Values

The toxicological reference values developed for alkanes, C11-15-iso- follow the methodology discussed in enHealth (2012). The approach used to develop drinking water guidance values is described in the Australian Drinking Water Guidelines (ADWG, 2011).

Non-Cancer

Oral

A 13-week oral gavage study was conducted on a C9-C14 aliphatic (<2% aromatic) hydrocarbon fluid in rats. There were no adverse effects at 5,000 mg/kg-day, the highest dose tested. Alternatively, two other tests indicate that the NOAEL for this substance is 1,000 mg/kg/day. Therefore, the NOAEL of 1,000 mg/kg-day will be used to derive the oral reference dose and the drinking water guidance value for alkanes, C11-15-iso-.

Oral Reference Dose (oral RfD)

Oral RfD = NOAEL / (UF_A x UF_H x UF_L x UF_{Sub} x UF_D)

Where:
UF_A (interspecies variability) = 10
UF_H (intraspecies variability) = 10
UF_L (LOAEL to NOAEL) = 1
UF_{Sub} (subchronic to chronic) = 3
UF_D (database uncertainty) = 1

Oral RfD = 5,000/(10 x 10 x 1 x 3 x 1) = 1,000/300 = 3.33 mg/kg-day

Drinking water guidance value

Drinking water guidance value = (animal dose) x (human weight) x (proportion of intake from water) / (volume of water consumed) x (safety factor)

Using the oral RfD,

Drinking water guidance value = (oral RfD) x (human weight) x (proportion of water consumed) / (volume of water consumed)

Where:
Human weight = 70 kg (ADWG, 2011)
Proportion of water consumed = 10% (ADWG, 2011)

Volume of water consumed = 2L (ADWG, 2011)

Drinking water guidance value = (3.33 x 70 x 0.1)/2 = 11.6 mg/L

Cancer

No carcinogenicity studies are available on C9-C14 aliphatic (<2% aromatic) hydrocarbon fluids. Thus, a cancer reference value was not derived for alkanes, C11-15-iso-.

K. Human Health Hazard Assessment Of Physico-Chemical Properties

Alkanes, C11-15-iso- do not exhibit the following physico-chemical properties:

- Explosivity
- Flammability
- Oxidising potential

7 ENVIRONMENTAL HAZARD ASSESSMENT

A. Summary

Alkanes, C11-15-iso- has a low acute toxicity concern to aquatic life.

B. Aquatic Toxicity

Acute Studies

Table 4 lists the results of acute aquatic toxicity studies conducted on hydrocarbons, C10-C12, isoalkanes (<2% aromatics).

Table 4 Acute Aquatic Toxicity Studies on C10-C12 Isoalkanes (<2% Aromatics)*

Test Substance	Test Species	Endpoint	Results (mg/L) [WAF]	Kl. score
Hydrocarbons, C10-C12, isoalkanes (<2% aromatics)	*Oncorhynchus mykiss*	96-hour LL_{50}	>1,000	1
Hydrocarbons, C10-C12, isoalkanes (<2% aromatics)	*Daphnia magna*	48-hour LL_{50}	>1,000	1
Hydrocarbons, C10-C12, isoalkanes (<2% aromatics)	*Pseudokirchnerella subcapitata*	72-hour LL_{50} 72-hour NOELR	>1,000 1,000	1

*All studies used the water accommodated fractions (WAFs) of the test substance.

Chronic Studies

The 28-day NOELR (No Observed Effect Loading Rate) for hydrocarbons, C11-13, isoalkanes (<2% aromatics) in freshwater fish is 0.316 mg/L based on growth. The value for NOELR was estimated by QSAR model – Petrotox. This model combines a partitioning model used to calculate the aqueous

concentration of hydrocarbon components with the Target Lipid Model used to calculate acute and chronic toxicity of non-polar narcotic chemicals. Petrotox computes toxicity based on the summation of the aqueous-phase concentrations of hydrocarbon block(s) that represent a hydrocarbon substance and membrane-water partition coefficients that describe the partitioning of the hydrocarbons between the water and organism (ECHA) [Kl. score = 2].

The 21-day NOELR for hydrocarbons, C11-13, isoalkanes (<2% aromatics) for *Daphnia* is 1 mg/L based on reproduction (ECHA) [Kl. score = 1].

C. Terrestrial Toxicity

No studies are available.

D. Calculation of PNEC

The PNEC calculations for alkanes, C11-15-iso- follow the methodology:

PNEC water

Using the QSAR model PETRORISK v7.04, the estimated $PNEC_{water}$ value for C11-15-iso- is 0.001 mg/L [Kl. score = 2].

PNEC sediment

Using the QSAR model PETRORISK, v7.04 the estimated $PNEC_{sediment}$ value for C11-15-iso- is 260 mg/kg soil wet weight (CONCAWE) [Kl. score = 2].

PNEC soil

Using the QSAR model PETRORISK v7.04, the estimated $PNEC_{sediment}$ value for C11-15-iso- is 100 mg/kg soil wet weight (CONCAWE) [Kl. score = 2].

8 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2017).

Based on the existing studies for similar substances, alkanes, C11-15-iso- is expected to be readily biodegradable. Thus, alkanes, C11-15-iso- does not the screening criteria for persistence.

Alkanes, C11-15-iso- is a UVCB substance. BCF values calculated for representative hydrocarbon structures in the group do not indicate a potential for bioaccumulation (BCF values <2,000). Thus, alkanes, C11-15-iso- does not meet the screening criteria for bioaccumulation.

Read-across substance hydrocarbons, C10-C12, isoalkanes (<2% aromatics) did not exhibit acute toxicity to fish, invertebrates or algae with measured toxicity values > 1 mg/L. Aquatic chronic

toxicity values were > 0.1 mg/L. Thus, alkanes, C11-15-iso- does not meet the screening criteria for toxicity.

The overall conclusion is that alkanes, C11-15-iso- is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for alkanes, C11-15-iso-.

9 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Alkanes, C11-15-iso-	90622-58-5	Not a PBT	No	No	No	No	No	No	1	2	2

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 - Tier 2 - Hazard Assessment and Qualitative Assessment Only. Develop toxicological profile and PNECs for water and soil and provide qualitative discussion of risk.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

10 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
BCFWIN	USEPA EPISuite model used to estimate bioconcentration factors
BCF	bioconcentration factor
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
ECHA	European Chemicals Agency
EPISUITE	Estimation Programs Interface Suite
EU	European Union
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilogram per cubic metre
KI	Klimisch scoring system
kPa	kilopascal
L	litre
L/kg	litres per kilogram
LC	lethal concentration
LD	lethal dose
LL	lethal level
mg/kg	milligrams per kilogram
mg/kg-day	milligrams per kilogram per day
mg/L	milligrams per litre
mg/m^3	milligrams per cubic metre
mm^2/s	square millimetres per second
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme
NOAEL	no observed adverse effect level
NOELR	no observed effect loading rate
OECD	Organisation for Economic Co-operation and Development
OTS	Office of Toxic Substances
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No Effect Concentration
ppm	parts per million
QSAR	quantitative structure activity relationship
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals

SD	Sprague Dawley
SGG	Synthetic Greenhouse Gases
USEPA	United States Environmental Protection Agency
UVCB	Unknown or Variable Composition, Complex Reaction Products and Biological Materials
WAF	water accommodated fraction